Qualitative Analysis of Low-lying Resonances of the Dipositronium Emerging from Ps-Ps and Ps-Ps* Collisions

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An analysis of the channel wave functions is made to clarify the types of resonance emerging from the Ps-Ps and Ps-Ps* collisions . The ordering of the energy levels of the states of the dipositronium is evaluated based on the inherent nodal structures of wave functions and on existing theoretical results. A few very probable low-lying narrower resonances, namely the $0_1^+(\mathrm{A}_2)$, $1_1^-(\mathrm{E})$,$\cdots$, benefiting from the centrifugal barrier have been proposed.

Since the discovery of the positron the investigation of the systems composed of positrons and electrons becomes an attractive topic. These systems might exist in astrophysical processes and might play an important role in astronomical evolution. Experimentally, the (e^+e^-) , $(e^+e^-e^-)$, and $(e^+e^+e^-)$ systems together with their excited states have long been found in laboratories. However, the $(e^+e^+e^-e^-)$ system, namely the dipositronium Ps_2, has not yet been found. Theoretically, in recent years the existence of the ground state of Ps_2 has been predicted by a number of authors[1−4], an excited bound state with $L^\Pi = 1^-$ (here L is the total orbital angular momentum, Π is the parity) has been predicted in the ref.[5], and two more excited bound 0^+ states have also been predicted in ref.[1,6]. Obviously, in addition to these bound states, resonances of Ps_2 might also exist, and they might emerge during Ps-Ps and Ps-Ps* collisions (here Ps and Ps* denote the ground state and the excited state, respectively, of the (e^+e^-) system). In this paper, a qualitative analysis is performed to evaluate what types of low-lying resonances might be observed during the above collisions.

Let us start from the Ps-Ps collision. Let the two positrons be called the particles 1 and 2, while the two electrons be 3 and 4. Let us assume that the spins of the positrons are coupled to s_1, and those of the electrons are coupled to s_2, and $\chi_{s_1 s_2}$ is the spin state. Let the spatial wave function of a Ps in its ground state be denoted as Φ. Then the antisymmetrized wave

function $\tilde{\Psi}$ of the Ps-Ps channel can be written as

$\Psi = \tilde{F}\ \chi_{s_1 s_2}$ (1)

where $\tilde{F}$ is a spatial wave function

$\tilde{F} = (1+(-1)^{s_1} p_{12})(1+(-1)^{s_2} p_{34})F$ (2)

where p_{ij} denotes an interchange of the indexes i and j, and

$F = \Phi(\overrightarrow{r_{13}})\Phi(\overrightarrow{r_{24}}) f_l(\overrightarrow{r}_{13,24})$ (3)

where $\overrightarrow{r_{13}} = \overrightarrow{r_3} - \overrightarrow{r_1}$, $\overrightarrow{r}_{13,24} = \frac{1}{2}(\overrightarrow{r_2} + \overrightarrow{r_4}) - \frac{1}{2}(\overrightarrow{r_1} + \overrightarrow{r_3})$, etc.; and $\overrightarrow{r_i}$ is the position vector of the i-th particle originating from the c.m.. f_l is for the relative motion of the two Ps with relative angular momentum l. Evidently, since the Ps are in their ground states, l is equal to the total orbital angular momentum L of the channel. From (1) to (3) we have

$\tilde{F} = (1+(-1)^{s_1+s_2+\mathrm{L}})[\Phi(\overrightarrow{r_{13}})\Phi(\overrightarrow{r_{24}}) f_L(\overrightarrow{r}_{13,24}) + (-1)^{s_1}\Phi(\overrightarrow{r_{23}})\Phi(\overrightarrow{r_{14}}) f_L(\overrightarrow{r}_{23,14})]$ (4)

It is obvious from (4) that the channel should have $s_1 + s_2 + \mathrm{L} = even$.

When L=even, it is clear from (4) that

$p_{13}p_{24}\ \tilde{F} = \tilde{F}$ (5)

Equation (5) implies that the spatial wave function $\tilde{F}$ of the channel should be invariant to $p_{13}p_{24}$ if L is even.

Furthermore, since the ground state of Ps has an even parity, the parity of the channel Π is therefore equal to $(-1)^l = (-1)^L$.

On the other hand, the eigenstates of the dipositronium Ps_2 can be classified by the rotation group, space inversion group, and D_{2d} point group[1,7]. Thus an eigenstate (bound state or resonance) can be labeled as $\mathrm{L}_i^{\Pi}(\mu)$, where μ denotes one of the representations A_1, A_2, B_1, B_2, and E of the D_{2d} group; the subscript i denotes the $i-th$ state of a series of states with the same L, Π,and μ . The $i = 1$ state is the lowest of the series. In some cases the subscript i may be omitted if it is not necessary to appear. Incidentally, μ is related to s_1 and s_2 as listed in Table 1[7]. Furthermore, when $\mu = A_1$ and B_1, the spatial wave function $\tilde{F}$ of the $\mathrm{L}_i^{\Pi}(\mu)$ states are invariant to $p_{13}p_{24}$; i.e., $\tilde{F}$ is an eigenstate of $p_{13}p_{24}$ with an eigenvalue $\Lambda = 1$. When $\mu = A_2$ and B_2, $\tilde{F}$ is also an eigenstate of $p_{13}p_{24}$ but with an eigenvalue $\Lambda = -1$.

Table 1

The relation between μ , s_1 and s_2, and Λ.

μ	A_1	B_2	B_1	A_2	E
(s_1, s_2)	(0,0)	(0,0)	(1,1)	(1,1)	(0,1) or (1,0)
Λ	1	-1	1	-1	

Evidently, the good quantum numbers of a resonance should match those of the channel wave functions. Thus, during the Ps-Ps collision, only the resonances with

(i) $s_1 + s_2$+L= *even*,

(ii) $\Lambda = 1$ if L is even,

(iii) parity $\Pi = (-1)^{\mathrm{L}}$

can be induced . Consequently, three types of resonances , namely the $\mathrm{L}_i^+(\mathrm{A}_1)$ states with an even L, the $\mathrm{L}_i^+(\mathrm{B}_1)$ states with an even L, and the $\mathrm{L}_i^-(\mathrm{E})$ states with an odd L, might emerge during Ps-Ps collision. It is noted that the observation of a resonance depends on its width. If the width is very broad, then the observation is difficult or even impossible. Therefore, the above three types of resonances might not all be observed.

The width of a resonance depends on how the wave function is distributed in the channel region and in the interior. If the amplitude of the wave function is small in the channel region (as to be compared with the amplitude in the interior), then the width is narrow and the state is nearly stable. If it is large in the channel region, then the width is broad. When the width is broad, the resonance is difficult to be identified and therefore might not be observed.

When the energy of a state is higher than the threshold of a channel and when the quantum numbers of the state match those of the channel, there are two factors to hinder the wave function in the interior from extending to the channel region. One is the difference in structure between the channel wave function and the wave function in the interior. When the difference is large, the extension of the wave function is difficult, and therefore the width is small. The other one is the centrifugal barrier and the Coulomb barrier. These barriers play their role only if the bombarding energy is low. Thus they are important to low-lying resonances in general. However, since the Ps and Ps* are neutral in charge, the Coulomb barrier is unimportant in our case, but the centrifugal barrier might be important. In what follows we shall study the effect of this barrier to the low-lying resonances.

Let us study the low-lying resonances with L$\leq$ 2 induced by Ps-Ps collision with the threshold energy -0.5 (atomic units are used in this paper). It has been calculated[1] that the energies of the $0_2^+(\mathrm{A}_1)$ and $0_1^+(\mathrm{B}_1)$ are -0.4995 and -0.4994, respectively . Both are a little higher than the Ps-Ps threshold and therefore they might be observed as resonances. However, since in this

case there is no centrifugal barrier to hinder the wave function, the widths of these two resonances might be broad. Thus, even if the calculation in the ref. [1] is correct, these resonances might not be observed.

The energy of the 1_1^-(E) state has never been calculated. Nonetheless, it was known from all existing theoretical calculations that the energy of a state would be high if the wave function contains many nodal surfaces; the more the nodal surfaces, the higher the energy. Besides, it was found that the first-states (the $i = 1$ states) either do not contain any nodal surface, or contain only the inherent nodal surfaces[8,9]. Thus the inherent nodal structures can be used to evaluate the ordering of the first-states. More specifically, for the dipositronium, the ordering of the $0_1^+(\mu)$ levels have been found to be just ordered according to the number of inherent nodal surfaces that they contain[7]. This fact should also be true for the group of other $\mathrm{L}_1^\Pi(\mu)$ states with L≠0. It was found[7] that the 1_i^-(E) states do not contain inherent nodal surfaces, while all the other L=1 states contain inherent nodal surfaces[7]. Thus the 1_1^-(E) state is the lowest L=1 state. It was calculated in the ref.[5] that the energy of $1_1^-(\mathrm{B}_2)$ is -0.3344. The energy of the 1_1^-(E) should be considerably lower than this value. If the energy of the 1_1^-(E) is lower than -0.5, then it is bound. If the energy is higher, then it is a resonance. It is noted that the first excited L=0 state and the lowest L=1 state of the positronium have exactly the same energy. This is in general not true for other systems. However, the energies of the $0_2^+(\mathrm{A}_1)$ and the 1_1^-(E) of the dipositronium might be close. If this is true, the energy of the 1_1^-(E) would be close to -0.4995 . On the other hand, the centrifugal barrier is equal to $\frac{l(l+1)}{2r^2} - 0.5$, where l is the relative partial wave of the two Ps, and r is the relative distance of the two Ps. Once the channel radius has been evaluated, the height of the barrier can be known. It is noted that the radius of a Ps is equal to 2, the channel radius should be considerably larger than this value. When the channel radius is given from 4 to 6, then the height of the $p-$wave barrier is from -0.4375 to -0.4722. So, if the energy of the 1_1^-(E) is considerably lower than the height of the barrier (e.g., the energy is close to -0.4995), the collapse of the state would be effectively hindered and accordingly the width would be narrower. In brief , there are three possibilities. If the energy of the 1_1^-(E) is lower than -0.5, the state is bound; if it is a little higher than -0.5, it is a narrow resonance and thereby can be easily observed; if it is much higher than -0.5, it might be a broad resonance and might not be observed.

The $2_i^+(\mathrm{A}_1)$ and $2_i^+(\mathrm{B}_1)$ states do not contain inherent nodal surfaces,

while the other $2_i^{\Pi}(\mu)$ states contain[7]. Thus the $2_1^+(\mathrm{A}_1)$ and $2_1^+(\mathrm{B}_1)$ states are the two lowest L=2 states. It is very unlikely that they would be lower than the threshold at -0.5, thus they are likely to be resonances. If their energies are considerably lower than the height of the $d-$wave barrier (e.g., their energies are lower than -0.46), they would have narrower widths and might be observed. Otherwise, the widths might be broad and the observation might be difficult.

In conclusion, the $1_1^-(\mathrm{E})$, $2_1^+(\mathrm{A}_1)$ and $2_1^+(\mathrm{B}_1)$ are possible narrower low-lying resonances that might emerge in Ps-Ps collision.

Let us study the low-lying resonances with L$\leq$ 2 induced by Ps-Ps*(2p) collision with the threshold energy -0.3125, here the excited Ps is in the (nl)=(2p) state. In this case the spatial part of the channel wave function reads

$$\widetilde{F}=\sum_l\{[\Phi(\overrightarrow{r_{13}})\Phi_{2p}(\overrightarrow{r_{24}}) + (-1)^{s_1+s_2+l}\Phi(\overrightarrow{r_{24}})\Phi_{2p}(\overrightarrow{r_{13}})]f_l(\overrightarrow{r_{13,24}})$$
$$+(-1)^{s_1}[\Phi(\overrightarrow{r_{23}})\Phi_{2p}(\overrightarrow{r_{14}}) + (-1)^{s_1+s_2+l}\Phi(\overrightarrow{r_{14}})\Phi_{2p}(\overrightarrow{r_{23}})]f_l(\overrightarrow{r_{23,14}})\}_L \qquad (6)$$

where Φ_{2p} is the wave function of the Ps*(2p) . When $(s_1, s_2) = (0, 0)$ or (1,1) , we have

$$p_{13}p_{24}\ \widetilde{F}= -\ \widetilde{F} \qquad (7)$$

Therefore, the Ps-Ps*(2p) channel can induce the $\mathrm{L}_i^{\Pi}(\mu)$ resonances with $\mu = A_2$ and B_2 (they have $\Lambda = -1$), and E. Furthermore, if L=0, we have $l = 1$ and $\Pi = +1$; therefore all the $0_i^-(\mu)$ resonances can not be induced.

For the case of L=0, the $p-$wave of the Ps-Ps*(2p) collision can induce the $0^+(\mathrm{E})$, $0^+(\mathrm{B}_2)$, and $0^+(\mathrm{A}_2)$ resonances. However, it was shown in the ref.[1] that the $0_1^+(\mathrm{E})$ and $0_1^+(\mathrm{B}_2)$ states are lower than the threshold, thus they can not be induced. Nonetheless, their higher states (e.g., the $0_2^+(\mathrm{E})$) might be observed if they are higher than and close to the threshold due to the $p-$wave barrier. The energy of the $0_1^+(\mathrm{A}_2)$ is -0.3121. Since the $0_1^+(\mathrm{A}_2)$ is only a little higher than the threshold, the p-wave barrier should act effectively. Thus the width of this resonance should be narrow and therefore can be easily observed. The search of this resonance is an interesting topic.

For the case of L=1, odd-parity resonances may be induced by s-wave while even-parity resonances can only be induced by p-wave. Thus, even-parity states in general might have a narrower width. Three kinds of even-parity states, namely the $1^+(\mathrm{A}_2)$, $1^+(\mathrm{B}_2)$, and $1^+(\mathrm{E})$, can be induced. It was found that the wave function of the $1^+(\mathrm{A}_2)$ is allowed by symmetry to be distributed surrounding a square with a pair of the same kind of particles located at the two ends of a diagonal (this geometric configuration is denoted as SQ), while the wave function of the $1^-(\mathrm{B}_2)$ is not allowed[7]. The SQ is the

most favorable configuration in favor of binding. Since the SQ is accessible to $1^+(A_2)$ but not accessible to $1^-(B_2)$, the $1_1^+(A_2)$ would be lower than the $1_1^-(B_2)$. The latter has an energy -0.3344, thus the former would be lower than the threshold and therefore might be bound. It was found[7] that the $1^+(B_2)$ and $1^+(E)$ contain more inherent nodal surfaces than the $1^-(B_2)$ contains. Thus the $1_1^+(B_2)$ and $1_1^+(E)$ would be higher than -0.3344. If their energies are higher than but close to the threshold -0.3125, they would have narrower widths and therefore might be observed. If they are much higher than the threshold, they would have a broad width and therefore difficult to be observed.

For the L=2 resonances, the bombarding wave should at least have $l = 1(2)$ if the parity is even (odd). Since the energies of L=2 states have never been evaluated, it is difficult to evaluate which resonances can be observed at this moment. Nonetheless, the odd parity resonances might have a larger possibility to be observed due to having a higher centrifugal barrier. Among the odd states the $2^-(B_2)$ and $2^-(A_2)$ should be very high due to having so many inherent nodal surfaces[7], while the $2^-(E)$ should be lower because the SQ is accessible to this state. If the $2_1^-(E)$ is lower than -0.3125, it is bound because the Ps-Ps channel is close to it; if it is higher than and close to -0.3125, it would be a resonance with a narrower width.

In conclusion, a number of $L_i^\Pi(\mu)$ resonances with $\mu = A_2$, B_2, and E might be induced in Ps-Ps*(2p) collision (among them the L=0 resonances have an even parity). Where the most probable narrower low-lying resonance is the $0_1^+(A_2)$. The existence of the other suggested narrower low-lying resonance, namely the $1_1^+(B_2)$, $1_1^+(E)$, and $2_1^-(E)$, is also possible

Let us study the low-lying resonances with L$\leq$ 2 induced by Ps-Ps*(2s) collision with also the threshold energy -0.3125. From an analysis similar to the above, $L^\Pi(\mu)$ resonances with $\Pi = (-1)^L$ and $\mu = A_1$, B_1, and E might be induced. However, the L=0 resonances do not contain centrifugal barrier, thus they have broad widths. The $1_1^-(A_1)$ and $1_1^-(B_1)$ contain many inherent nodal surfaces just as the $0_1^+(A_2)$ state[7], but the energies of the former two should be considerably higher than the latter (at -0.3121) due to the difference in L, thus the former should be considerably higher than the threshold -0.3125. Thus they can not take advantage from the $p-$wave barrier, and therefore have a broad width. The $1_1^-(E)$ has been mentioned that it might appear as a narrower resonance emerging from Ps-Ps collision. It is possible that the $1_2^-(E)$ resonance might be observed during the Ps-Ps*(2s) collision. Among the L=2 states, the $2_1^+(E)$ has the same inherent nodal structure just as the $1_1^-(B_2)$[7]. The former should considerably higher

than the latter (at -0.3344) due to the difference in L, but may not much higher than the threshold -0.3125. Thus the 2_1^+(E) may take advantage from the $d-$ wave barrier and therefore has a narrower width, and thereby can be observed.

In summary, an analysis based on symmetry has been performed in this paper. Which types of resonance would emerge during the Ps-Ps and Ps-Ps* collisions is clarified via the analysis of the channel wave functions. The ordering of the energy levels of the states of the dipositronium is evaluated based on the inherent nodal structures of wave functions and on existing theoretical results. How the widths are affected by the centrifugal barrier has been discussed. Emphasis is placed on the states that might have an energy higher than and close to the Ps-Ps or Ps-Ps* threshold. A few very probable low-lying narrower resonances benefiting from the centrifugal barrier have been proposed. The existence of these suggested narrower resonances remain to be checked.

Although the above qualitative analysis can only talk about the possibilities but does not give definite quantitative results, the analysis is still useful because it can help us to understand the physics underlying the forthcoming experimental data and theoretical results. Specificallly, as a first step, the experiment for the identification of the $0_1^+(\mathrm{A}_2)$ resonance via the Ps-Ps*(2p) collision is suggested. If this resonance can not be found, this state would be the fifth bound state (together with the $0_1^+(\mathrm{A}_1)$,0_1^+(E), $0_1^+(\mathrm{B}_2)$, and $1_1^-(\mathrm{B}_2)$ that have been theoretically confirmed to be bound).

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